

NOVA

NERSC's Online VASP Application

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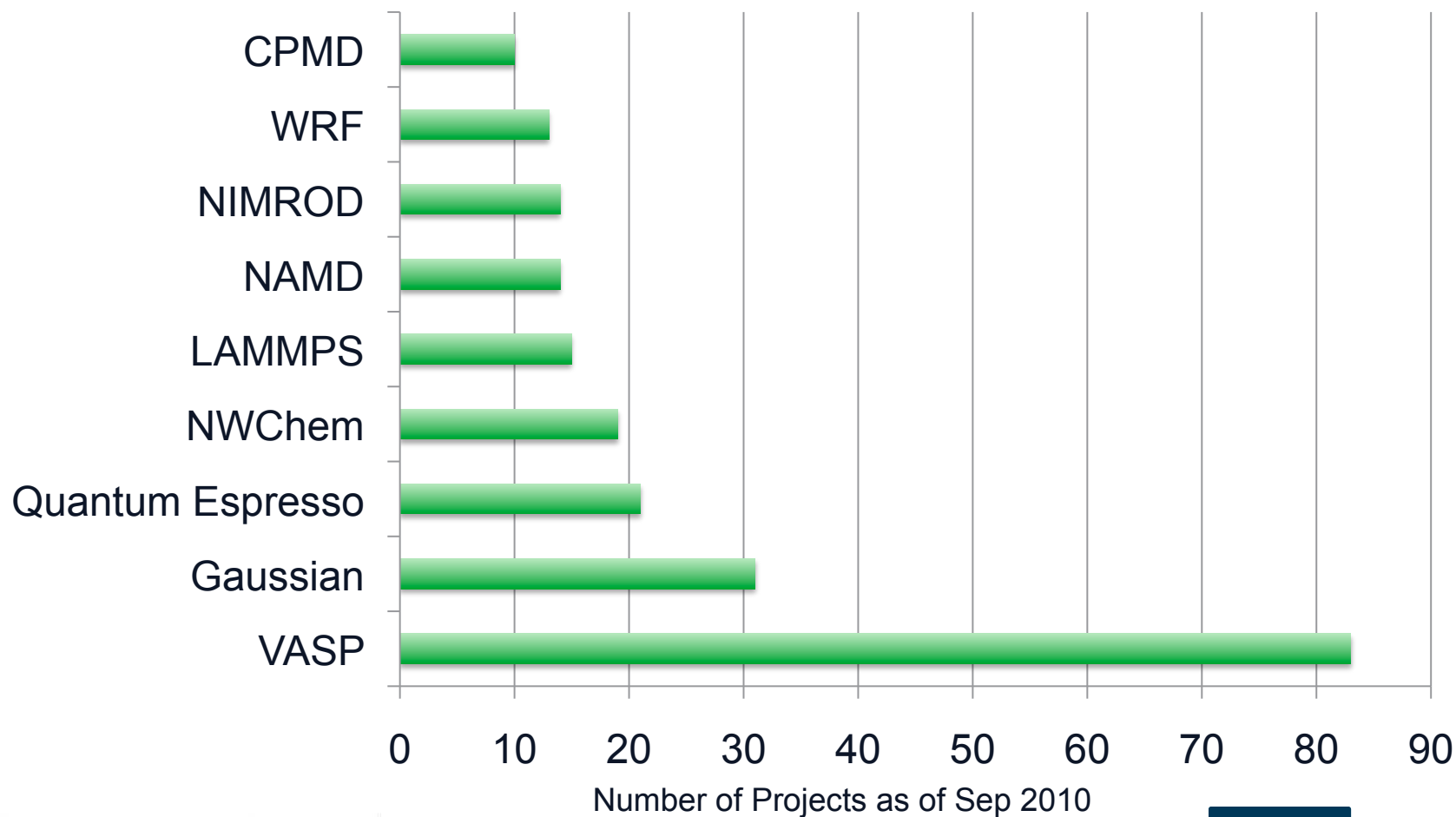


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Why VASP?

Codes Used by the Most Projects at NERSC



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Why run VASP in a browser?

Making interacting with HPC more efficient

- Error checking
- Organizing and retrieving jobs
- Real-time job monitoring
- Integrated analysis tools
- Integration with other online tools
- Meaningful UI controls



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VASP with a modern interface

```
SYSTEM = Hg

NWRITE = 2
IALGO = 48 ! uncomment this line to get timings
NELM = 13
ENMAX = 140 eV ; IALGO = -1 ; NELMIN = 3 ; NELMDL = 7
NGX=31 ; NGY=31 ; NGZ=31 ; NGXf=48 ; NGYf=48 ; NGZf=48
NBANDS=316
NSIM =4

LREAL = .TRUE.    real space projections
BMIX  = 2.5       mixing parameter
ISYM  = 0         switch of symmetry
EDIFF = 1E-4
LWAVE=.FALSE.
LCHARG=.FALSE.

Ionic Relaxation
NSW    = 0        number of steps for IOM
NBLOCK = 1 ; KBLOCK = 5
SMASS  = 0.5      Nose mass-parameter (am)
POTIM  = 5.00     time-step for ion-motion
TEBEG  = 423      temperature

PC-function
APACO  = 10.0     distance for P.C.

Mass of Ions in am
POMASS = 200.59000
ZVAL   = 12.00
```



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VASP with a modern interface

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NERSC NOVA Job Control

[VASP Manual Window](#)

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Files

[POSCAR](#)
[POTCAR](#)
[KPOINTS](#)
[INCAR](#)

Computational Settings

Run this job

☐ Graphical ☒ [Raw Text](#)

Recommended Minimal Settings

Precision:	<input type="text" value="Normal"/>	PREC
Cutoff energy for plane wave basis set:	<input type="text" value="500"/>	ENCUT
Projection done in:	<input type="text" value="Reciprocal space"/>	LREAL
Method to determine partial occupancies:	<input type="text" value="Tetrahedron method with Blochl corrections (-5)"/>	ISMEAR
Order:	<input type="text"/>	

[+ Optional Initialization Settings](#)
[+ Optional Iteration Settings](#)
[+ Optional Quality Settings](#)
[+ Optional Algorithm Settings](#)



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+ Optional Initialization Settings

- Optional Iteration Settings

Max number of electronic steps:	<input type="text" value="61"/>	NELM
Min number of electronic steps:	<input type="text" value="6"/>	NELMIN
Max number of ionic steps:	<input type="text" value="51"/>	NSW
Calculate pair correlation function and DOS each <input type="text"/>	ionic steps	NBLOCK
Max number of steps in Broyden mixer:	<input type="text"/>	MAXMIX
	<input type="checkbox"/> Only reset if storage exceeded	
Begin updating charge density	<input checked="" type="radio"/> according to default <input type="radio"/> immediately <input type="radio"/> after <input type="text"/> steps, <input type="checkbox"/> with delay after each ionic step	NELMDL



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Files

[POSCAR](#)
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[INCAR](#)

Computational Settings

Run this job

Computational Settings

VASP version: 4.6.35 - default

VASP executable: collinear (vasp) - default

Queue: regular

Run On: 1 nodes x 8 procs per node = 8 cores

Maximum Walltime: Hours Minutes

Node Memory: First Available

Process Memory Limit: GB

Email Notifications:
☐ On begin
☐ On end
☐ On abort

Repository: Default

[Save](#) [Cancel](#)



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Job Control

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Job Control

New Job

Import
Job

Jobs to Be Run

Oxygen in a box [[View All Files](#)] [[Copy Job](#)]

Jobs Running

Li O Al [[View All Files](#)] [[Copy Job](#)] [[Stop Job](#)]
Queued April 3, 2011, 8:12 p.m.
Not yet started.

Jobs Recently Completed

Oxygen Atom in a Box [[View Convergence](#)] [[View All Files](#)] [[Copy Job](#)]
Started April 3, 2011, 2:58 p.m.
Completed April 3, 2011, 2:58 p.m.



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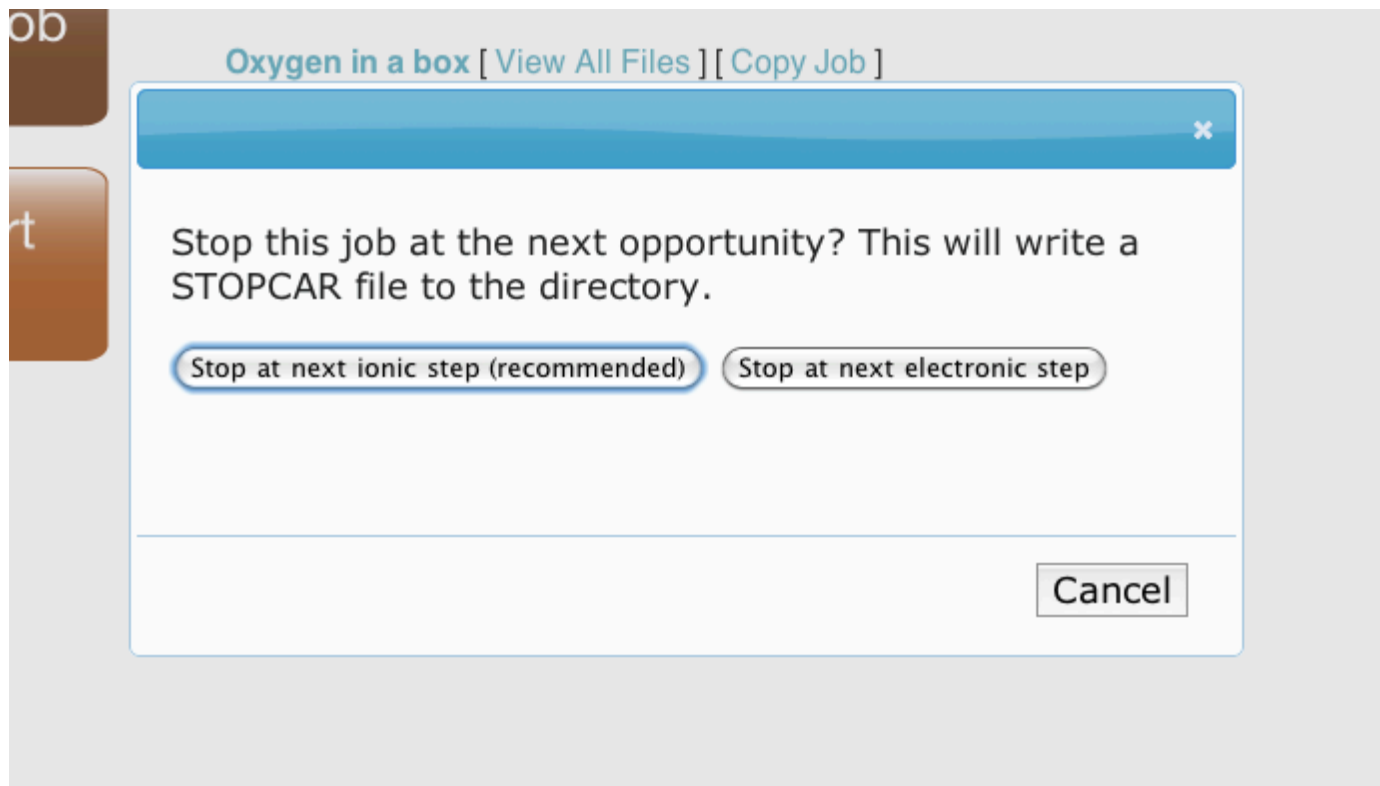
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Real-Time Monitoring



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Real-Time Monitoring

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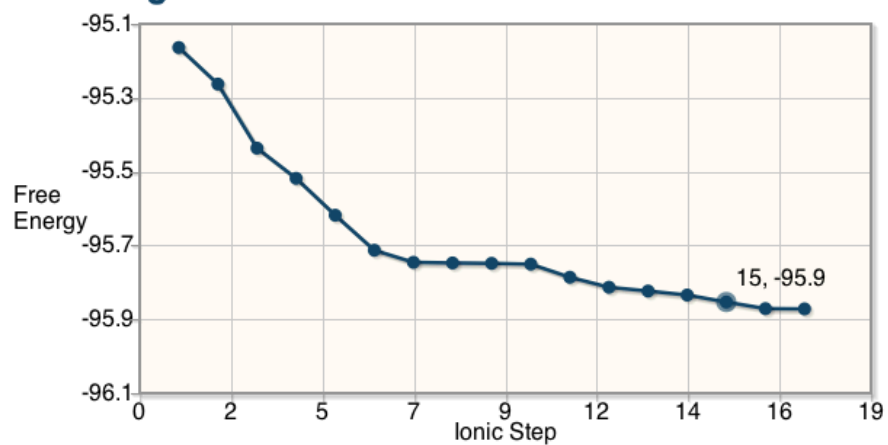
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Job Control

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Convergence



Job Information

System: carver

PBS Job ID: 606410.cvrsvc09-ib



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Current State of NOVA

- Django application using the NEWT API
- Early version implements some graphical features
- Checks INCAR keywords and values
- Can set up jobs, copy, submit, monitor, stop, import files from outside NOVA



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Future Features

- Real-time convergence monitoring
- POSCAR file generation
- Ensured coherency across input files
- Visualization tools
- Advanced error detection
- File sharing
- Connection to Materials Genome Project



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Available April 11

Test version of NOVA

<https://portal-auth.nersc.gov/nova>

Comments and suggestions to
amgreiner@lbl.gov



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